

Trace Formulae for quantum graphs with edge potentials

Ralf Rueckriemen¹ and Uzy Smilansky^{1,2}

¹School of Mathematics, Cardiff University, Cardiff CF24 4AG, Wales, UK

²Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel.

Abstract. This work explores the spectra of quantum graphs where the Schrödinger operator on the edges is equipped with a potential. The scattering approach, which was originally introduced for the potential free case, is extended to this case and used to derive a secular function whose zeros coincide with the eigenvalue spectrum. Exact trace formulas for both smooth and δ -potentials are derived, and an asymptotic semiclassical trace formula (for smooth potentials) is presented and discussed.

1. Preliminaries and a summary of the main results

A metric graph is a finite combinatorial graph where each edge is endowed with the natural metric and with a positive real length. A quantum graph is a metric graph together with a Schrödinger operator acting on it. The operator acts as second derivative plus lower order parts on the individual edges. Boundary conditions are imposed at the vertices to ensure that the operator is self adjoint. Quantum graphs were first introduced in the 1930s by Pauling to study the movement of electrons in molecules. They are a popular model for various physical processes involving wave propagation. The survey articles [GS06], [Kuc08] and [Pos09] provide an excellent overview.

One of the key properties that make quantum graphs such a useful model is the existence of an exact trace formula. The first trace formula for quantum graphs was proved in [Rot84]. It is valid for the standard Laplacian with Kirchhoff-Neumann boundary conditions at the vertices. Various generalizations have been shown, valid for Schrödinger operators with a magnetic field and much more general boundary conditions, (see [KS99b, KPS07, BE09] or [BE08] for a survey). However, all of these rely on the fact, that the eigenvalue equation can be solved explicitly on each of the individual edges, the eigenfunctions are linear combinations of counter-propagating free waves.

Here, we consider the case of a more general Schrödinger operator $\Delta + w$ where w stands for the set of edge potentials, as will be detailed below. In this case the solutions on the edges are no longer known explicitly. However, Sturm-Liouville theory still guarantees the existence of two independent solutions on each edge. In the high energy limit these solutions converge to the freely propagating waves of the no potential

setting (see for example [PT87]). Quantum graphs with a potential are also considered in [GS06], [CS07] and [HKT12]. Their methods are complementary to ours and the focus is on different aspects of the problem.

Before stating our main results we provide some necessary definitions and describe the model.

1.1. The model

Let \mathcal{G} be a graph defined by a vertex set \mathcal{V} and an edge set \mathcal{E} . Their respective cardinalities will be denoted by $V = |\mathcal{V}|$ and $E = |\mathcal{E}|$. The natural Euclidean measure is attributed to the edges, and the length of an edge is denoted by L_e , for $e \in \mathcal{E}$. The number of edges and vertices as well as the length of each edge are assumed to be finite. Distance along an edge can be measured from either of the connected vertices, and it is convenient to use a directed edge notation to specify the direction of increasing coordinate. Thus, given an edge $e \in \mathcal{E}$, one defines the two corresponding directed edges denoted by d and \hat{d} . The set of directed edges will be denoted by \mathcal{D} . The initial and terminal vertices of a directed edge $d \in \mathcal{D}$ will be denoted by $\iota(d)$ and $\tau(d)$, respectively. Clearly $\iota(d) = \tau(\hat{d})$. The coordinate on the directed edge will be denoted by x_d and it assumes the value 0 at $\iota(d)$ and L_d at $\tau(d)$. Thus, $x_d = L_d - x_{\hat{d}}$. It is convenient to associate the length to the directed bonds, in which case $L_d = L_{\hat{d}} = L_e$.

The Schrödinger operator on each directed edge is defined as the sum of the (magnetic) Laplacian and a real continuous potential $w_d(x)$:

$$\Delta_{w,A} := - \left(\frac{\partial}{\partial x_d} - iA_d \right)^2 + w_d(x), \quad \text{with } d \in \mathcal{D}. \quad (1)$$

Here A_d are the position independent “magnetic potentials” associated to each edge with $A_d = -A_{\hat{d}}$. For simplicity of exposition, it will be assumed that $A_d = 0$ on all edges, the generalization is straight forward. Denote the operator $\Delta_{w,0} = \Delta_w$. Clearly, $w_d(x) = w_{\hat{d}}(L_e - x)$. The edge operator acts on the space of twice differentiable complex valued functions in the interval $[0, L_e]$. It is natural to define the edge potentials to be continuous on all the vertices: $w_d(0) = w_{d'}(0)$ for all $d, d' : \iota(d) = \iota(d')$.

The graph Schrödinger operator acts on $2E$ dimensional vectors $(\psi_d(x))_{d \in \mathcal{D}}$. To get a consistent description, they are invariant under a switch of the preferred direction on the edges, $\psi_d(x) = \psi_{\hat{d}}(L_d - x)$. The bond wave functions are continuous at the vertices and are doubly differentiable in $(0, L_d)$. The Schrödinger operator is self adjoint if appropriate boundary conditions are chosen at the vertices. For the sake of clarity of notation, only the Kirchhoff-Neumann boundary conditions will be used:

$$\sum_{d \in \mathcal{D}: \iota(d)=v} \left. \frac{\partial \psi_d}{\partial x_d} \right|_{x_d=0} = 0 \quad \forall v \in \mathcal{V}. \quad (2)$$

The formalism can be easily extended to include other types of boundary conditions as in [KS99a].

It is instructive to recall the main steps taken to derive the trace formula and point out the differences and similarities between the no potential case as done in [KS97] and [KS99b] and the potential case here.

On every directed edge d the eigenvalue equation

$$-\psi_d''(x) + w_d(x)\psi_d(x) = k^2\psi_d(x) \quad (3)$$

has two independent solutions, denoted by ψ_d^+ and ψ_d^- . Normalize them so that

$$\psi_d^\pm(0) = 1 \quad (\psi_d^\pm)'(0) = \mp ik \quad (4)$$

This corresponds to the two solutions $e^{\mp ikx}$ in the no potential setting, where the sign convention is made so that ψ_d^+ is the incoming wave and ψ_d^- is the outgoing wave. The general solution is then given by

$$\psi_d(x) = a_d\psi_d^+(x) + b_d\psi_d^-(x) \quad (5)$$

Finding an eigenfunction on the entire graph is now equivalent to finding a list of coefficients a_d and b_d . These coefficients have to satisfy two types of conditions:

First, they have to be invariant under a switch of orientation on each edge. The general solution on the edge e can be rewritten in terms of $\psi_{\hat{d}}^+$ and $\psi_{\hat{d}}^-$, the two solutions on the same edge with reversed orientation.

$$\psi_d(L_e - x) = \psi_{\hat{d}}(\hat{x}) = a_{\hat{d}}\psi_{\hat{d}}^+(\hat{x}) + b_{\hat{d}}\psi_{\hat{d}}^-(\hat{x}) \quad (6)$$

Here \hat{x} traverses the edge in the opposite direction.

The resulting linear relation is captured in the edge transition matrix $t^{(e)}(k; w_e)$ defined by:

$$\begin{pmatrix} a_d \\ a_{\hat{d}} \end{pmatrix} = t^{(e)}(k; w_e) \begin{pmatrix} b_{\hat{d}} \\ b_d \end{pmatrix} \quad (7)$$

The matrix $t^{(e)}(k; w_e)$ is unitary, it depends on the potential on the edge and on k . It will be derived explicitly in section 2. If there is no potential the edge transition matrix describes the phase shift acquired by free propagation along the edge, and $t^{(e)}(k; 0)$ is a diagonal matrix with equal diagonal entries e^{ikL_e} . If there is a potential, there will be both transmission and reflection on the edge, and the edge transition matrix is not necessarily diagonal.

Second, the eigenfunctions have to satisfy the boundary conditions at all the vertices, this step is equivalent to the no potential case and is captured in the vertex scattering matrices σ^v .

$$b_d = \sum_{d': \tau(d')=v} \sigma_{dd'}^v a_{d'} \quad (8)$$

where $\iota(d) = v$. In physical terms, σ^v describes the scattering of waves at a vertex v as dictated by the vertex boundary conditions. For the Kirchhoff-Neumann boundary conditions it reads,

$$\sigma_{dd'}^v = -\delta_{d,d'} + \frac{2}{\deg(v)}, \quad \text{for } \tau(d') = \iota(d) = v \quad (9)$$

where $\deg(v)$ is the degree (valency) of the vertex v and δ is the Kronecker- δ . Note that the scattering from an incoming edge to all outgoing edges is the same except for the scattering back to the same edge.

The vertex scattering matrices are the building blocks for construction of the $2E \times 2E$ matrix

$$\Sigma_{dd'} = \delta_{\tau(d'), \iota(d)} \sigma_{dd'}^v \quad \text{where } v = \iota(d) . \quad (10)$$

In a similar way, the graph transition matrix $T(k; w)$ is constructed from the edge transition matrices

$$T_{dd'}(k; w) = (\delta_{\hat{d}, d'} + \delta_{d, d'}) t_{dd'}^{(e)}(k; w_e), \quad \text{where } e = (\iota(d), \tau(d)) . \quad (11)$$

1.2. The main results

Putting all the above conditions and definitions together, gives rise to the *secular function* $\zeta_w : \mathbb{C} \rightarrow \mathbb{C}$. The first main result of this work states its explicit form:

Theorem 1.1.

Let \mathcal{G} be a metric graph with the Schrödinger operator Δ_w . Then there exists a secular function of the form

$$\zeta_w(k) = (\det S_w(k))^{-\frac{1}{2}} \det(Id_{2E} - S_w(k)), \quad \text{where} \quad S_w(k) = \Sigma T(k; w) , \quad (12)$$

whose zeros correspond to the eigenvalues of the operator including multiplicities (with the possible exception of the eigenvalue zero).

Note that the secular function is of the same form as in the no potential case, see for example [KS99b]. The vertex scattering matrix Σ is identical. The key difference is in the transition matrix $T(k; w)$. If there is no potential this is a diagonal matrix which takes care of the phase shift accumulated when the wave propagates from one end of an edge to the other. In the present setting it is not necessarily diagonal, and it describes the transmission and the reflection induced by the edge potential.

The Cauchy argument principle can be applied to count the zeros of the secular function (12) and to derive a trace formula. However, before this is done, the concept of periodic orbits on the graph should be re-examined.

In general, a periodic orbit is a closed oriented walk on the graph. It is completely determined by the topology (connectivity) of the graph. The periodic orbits on a potential free quantum graph coincide with the topological periodic orbits. However, in the presence of an edge potential, a classical particle or a wave is not only transmitted through the edge but can also be reflected back. Thus, a periodic orbit can include back-scattering from the edge potential - a dynamically induced variant which is not accounted for by the topology. In order to systematically include the possibility of potential induced reflections, the following scheme is proposed. It makes use of an auxiliary graph denoted by \mathcal{G}^* . It is created from the original graph \mathcal{G} by inserting an auxiliary vertex (of degree 2) on each edge. The resulting graph is bipartite. Now, the reflection and transmission induced by the 2×2 transition matrices $t^{(e)}(k; w_e)$ can

be formally considered as the vertex scattering matrix of the corresponding auxiliary vertex. The set of periodic orbits in the trace formula is then the topological set of periodic orbits on \mathcal{G}^* , which will be denoted by PO^* . This is a new feature due to the edge potentials that does not occur in the free setting.

The trace formula is a formal equality between distributions. To give it a meaning as a functional equality, a suitable space of test functions is required. Throughout, test functions are denoted by φ , it is assumed they are analytic on the real line, admit a holomorphic extension to a neighbourhood of the real line and are rapidly decreasing.

The second main result of the present work is given in the following theorem.

Theorem 1.2.

Let \mathcal{G} be a metric graph with Schrödinger operator Δ_w . Denote its positive eigenvalues by $\{k_n^2\}_n$. Then there exists $K \geq 0$ such that

$$\sum_{k_n > K}^\infty \varphi(k_n) = \frac{1}{2\pi} \int_K^\infty \varphi(k) \frac{\partial \Theta_w(k)}{\partial k} dk + \frac{1}{\pi} \text{Im} \int_K^\infty \varphi(k) \sum_{p \in PO^*} \mathcal{A}_p(k) dk \quad (13)$$

for all test functions φ . The phase of $\det T(k; w)$ is denoted by $\Theta_w(k)$. The $\mathcal{A}_p(k)$ are complex amplitudes associated to each periodic orbit. They are build from elements of the matrix $S_w(k)$ along the periodic orbit, the explicit formula is written down in (43).

The threshold K depends on the edge potentials and it is a necessary ingredient in the theory. Its origin will be explained both in the formal proof of the theorem and in the example where the trace formula for δ -potentials is derived. The trace formula (13) is exact and the coefficients $\Theta_w(k)$ and $\mathcal{A}_p(k)$ depend implicitly on the potential. For high energies the eigenfunctions converge to the free solutions. Thus to leading order in k the trace formula above converges to the no potential case. Indeed, in the potential free case, $K = 0$, $\Theta_0(k) = 2k\mathcal{L}$, where $\mathcal{L} = \sum_{e \in \mathcal{E}} L_e$ and the leading order part of $\mathcal{A}_p(k)$ depends only on the vertex scattering matrix Σ and the edge lengths. Using the WKB-approximation it is also possible to compute the first order correction term. The resulting semi-classical trace formula will be discussed in the last section of the present work.

The rest of the paper is arranged as follows. In section 2 the transition matrix for a single edge $t(k; w)$ will be explicitly derived, and its relevant properties will be discussed. Using this information, the proof of the two main theorems will follow in section 3. The construction will be illustrated in section 4 by considering a simple system with a δ -potential on the edges. Finally, the asymptotic semi-classical trace formula will be derived in section 5.

2. The transition matrix for a single edge

Consider a single edge e of the quantum graph. As explained in section 1.1 the general solution of the eigenvalue equation can be expressed in two different ways corresponding to the different orientations of the edge.

$$a_d \psi_d^+(x) + b_d \psi_d^-(x) = a_{\bar{d}} \psi_{\bar{d}}^+(L - x) + b_{\bar{d}} \psi_{\bar{d}}^-(L - x) \quad (14)$$

Recall the definition of the edge transition matrix.

Definition 2.1.

The edge transition matrix $t^{(e)}(k; w_e)$ is defined by the equation

$$\begin{pmatrix} a_d \\ a_{\hat{d}} \end{pmatrix} = t^{(e)}(k; w_e) \begin{pmatrix} b_{\hat{d}} \\ b_d \end{pmatrix} \quad (15)$$

Using the symbol $'$ to denote differentiation with respect to x , equation (14) implies

$$\psi_d(0) = \psi_{\hat{d}}(L) \quad \psi_d'(0) = -\psi_{\hat{d}}'(L) . \quad (16)$$

A direct computation then yields an explicit expression for the transition matrix.

Lemma 2.2.

The transition matrix is given by

$$t^{(e)}(k; w_e) = \frac{1}{\psi_d^+(0)(\psi_{\hat{d}}^+)'(L) + (\psi_d^+)'(0)\psi_{\hat{d}}^+(L)} \cdot \begin{pmatrix} -W(\psi_d^+, \psi_{\hat{d}}^-) & -\psi_{\hat{d}}^-(0)(\psi_d^+)'(L) - (\psi_{\hat{d}}^-)'(0)\psi_d^+(L) \\ -\psi_d^+(0)(\psi_{\hat{d}}^-)'(L) - (\psi_d^+)'(0)\psi_{\hat{d}}^-(L) & -W(\psi_d^+, \psi_{\hat{d}}^-) \end{pmatrix} \quad (17)$$

where $W(\psi_d^+, \psi_{\hat{d}}^-) = \psi_d^+(\psi_{\hat{d}}^-)' - (\psi_d^+)' \psi_{\hat{d}}^-$ is the Wronskian.

In order to derive the trace formula the matrix $t^{(e)}(k; w_e)$ needs to be unitary on the real line. This is achieved through the choice of a suitable normalization of ψ_d^+ and $\psi_{\hat{d}}^-$. The matrix $t^{(e)}(k; w_e)$ is unitary on the real line whenever

$$\psi_d^+(0) = \overline{\psi_{\hat{d}}^-(0)} \quad (18)$$

which is satisfied with the normalization $\psi_d^\pm(0) = 1$ and $(\psi_d^\pm)'(0) = \mp ik$. Note that the potential is real, so the system has two real solutions, hence $\psi_d^+(x) = \overline{\psi_{\hat{d}}^-(x)}$ for all points on the interval. It also implies that $W(\psi_d^+, \psi_{\hat{d}}^-) \in i\mathbb{R}$ and $|\psi_d^+| = |\psi_{\hat{d}}^-|$.

The eigenvalues of $t^{(e)}(k; w_e)$ are

$$\mu_{1,2} = -\frac{W(\psi_d^+, \psi_{\hat{d}}^-) \pm |\psi_{\hat{d}}^-(0)(\psi_d^+)'(L) + (\psi_{\hat{d}}^-)'(0)\psi_d^+(L)|}{\psi_d^+(0)(\psi_{\hat{d}}^+)'(L) + (\psi_d^+)'(0)\psi_{\hat{d}}^+(L)} \quad (19)$$

For the derivation of the trace formula it is necessary to have control of the behaviour of $t^{(e)}(k; w_e)$ in the vicinity of the real k axis. This is done in using the following lemma.

Lemma 2.3.

For any given potential $w_e \in L^2([0, L])$ there exist a K such that the matrix $t^{(e)}(k+i\varepsilon; w_e)$ is sub-unitary for $k > K$ and $\varepsilon > 0$.

For high energies the matrix $t^{(e)}(k; w_e)$ converges to the no potential case.

$$t^{(e)}(k; w_e) = \begin{pmatrix} e^{ikL} & 0 \\ 0 & e^{ikL} \end{pmatrix} + O(k^{-1}) \quad (20)$$

Proof. Take k real. From standard properties of Sturm-Liouville problems, [PT87], the two solutions ψ^\pm satisfy

$$\begin{aligned} |\psi^\pm(x) - e^{\mp ikx}| &< \frac{2}{k} e^{\|w\|_{L^2} \sqrt{L}} \\ |(\psi^\pm)'(x) \mp ike^{\mp ikx}| &< 2\|w\|_{L^2} e^{\|w\|_{L^2} \sqrt{L}} \end{aligned} \quad (21)$$

and

$$\begin{aligned} \frac{\partial \psi^\pm}{\partial k}(x) &= -i \int_0^x \psi^\pm(\tilde{x}) (\psi^+(x)\psi^-(\tilde{x}) - \psi^+(\tilde{x})\psi^-(x)) d\tilde{x} \\ &\quad \mp \frac{1}{2k} (\psi^+(x) - \psi^-(x)) \\ \frac{\partial (\psi^\pm)'}{\partial k}(x) &= -i \int_0^x \psi^\pm(\tilde{x}) ((\psi^+)'(x)\psi^-(\tilde{x}) - \psi^+(\tilde{x})(\psi^-)'(x)) d\tilde{x} \\ &\quad \mp \frac{1}{2k} ((\psi^+)'(x) - (\psi^-)'(x)) \end{aligned} \quad (22)$$

Define an error function $E(x, k)$ via

$$\psi^+(x) = e^{-ikx} + E(x, k) \quad \psi^-(x) = e^{ikx} + \overline{E(x, k)} \quad (23)$$

then the bounds above imply

$$\begin{aligned} |E(x, k)| &< \frac{C}{k} & |E'(x, k)| &< C \\ \left| \frac{\partial}{\partial k} E(x, k) \right| &< \frac{C}{k} & \left| \frac{\partial}{\partial k} E'(x, k) \right| &< C \end{aligned} \quad (24)$$

for some constant C depending on the potential but independent of k and $x \in [0, L]$. Plugging (23) in the transition matrix yields

$$\begin{aligned} t^{(e)}(k; w_e) &= \frac{1}{e^{-ikL} - \frac{1}{2ik} (E'(L, k) - ikE(L, k))} \\ &\quad \cdot \begin{pmatrix} 1 & \frac{1}{2ik} (E'(L, k) + ikE(L, k)) \\ \frac{1}{2ik} (\overline{E'(L, k)} - ik\overline{E(L, k)}) & 1 \end{pmatrix} \end{aligned} \quad (25)$$

This implies

$$t^{(e)}(k; w_e) = \begin{pmatrix} e^{ikL} & 0 \\ 0 & e^{ikL} \end{pmatrix} + O(k^{-1}) \quad (26)$$

as claimed. The eigenvalues of $t^{(e)}(k; w_e)$ are given by

$$\begin{aligned} \mu_{1,2}(k) &= \frac{1 \pm \frac{1}{2ik} |E'(L, k) + ikE(L, k)|}{e^{-ikL} - \frac{1}{2ik} (E'(L, k) - ikE(L, k))} \\ &= e^{ikL} + \frac{1}{2ik} \frac{e^{ikL} (E'(L, k) - ikE(L, k)) \pm |E'(L, k) + ikE(L, k)|}{e^{-ikL} - \frac{1}{2ik} (E'(L, k) - ikE(L, k))} \end{aligned} \quad (27)$$

Let

$$\tilde{E}_{1,2}(k) := \frac{1}{2ik} \frac{e^{ikL} (E'(L, k) - ikE(L, k)) \pm |E'(L, k) + ikE(L, k)|}{e^{-ikL} - \frac{1}{2ik} (E'(L, k) - ikE(L, k))} \quad (28)$$

then

$$\left| \tilde{E}_{1,2}(k) \right| < \frac{\tilde{C}}{k} \quad \left| \frac{\partial}{\partial k} \tilde{E}_{1,2}(k) \right| < \frac{\tilde{C}}{k} \quad (29)$$

from the bounds on $E(L, k)$ and $E'(L, k)$. Here \tilde{C} can be computed from C , it also depends on the potential but not on k or x .

Thus

$$\frac{\partial}{\partial \varepsilon} \bigg|_{\varepsilon=0} |\mu_{1,2}(k + i\varepsilon)|^2 = -2L + O(k^{-1}) \quad (30)$$

which is smaller than zero for large enough values of k . \square

Remark 2.4.

This lemma still holds in the case of a δ -potential as will be shown in section 4. While one could use this lemma to derive an explicit bound for K the resulting bound would be very crude.

In the case of no potential or a positive δ -potential one can choose $K = 0$. For a negative δ -potential the transition matrix $t^{(e)}(k; w_e)$ is not subunitary above the real axis for small values of k and an explicit value for the optimal value of K will be computed.

3. The secular equation and trace formula for graphs with edge potentials

We will now derive the secular function ζ_w for a quantum graph with potential. Each edge will be treated as a scatterer similar to the vertices, using the transition matrix derived in the previous section. The matrix Σ controls the scattering at the vertices of the graph, and it is not affected by the introduction of the potential. On all the vertices Kirchhoff-Neumann boundary conditions are imposed.

Using the $2E \times 2E$ matrices Σ and $T(k; w)$ (10,11) we recall

$$S_w(k) := \Sigma \cdot T(k; w) . \quad (31)$$

Now the conditions on the coefficients a_d and b_d can be written as

$$S_w(k) \begin{pmatrix} b_1 \\ \vdots \\ b_D \end{pmatrix} = \begin{pmatrix} b_1 \\ \vdots \\ b_D \end{pmatrix} \quad (32)$$

In other words, the eigenvalues of Δ_w on the graph correspond to the values of k where $S_w(k)$ has eigenvalue 1, including multiplicities. The eigenvector defines the eigenfunction in terms of the ψ^\pm . This argument does not hold for $k = 0$ as the functions ψ^\pm are not linearly independent with our normalization.

Note that $S_w(k)$ is unitary on the real axis and subunitary above the real axis for large enough values of k by lemma 2.3 and the fact that Σ is unitary and independent of k .

To prove theorem 1.1 recall the definition (12) of the secular function

$$\zeta_w(k) := (\det S_w(k))^{-\frac{1}{2}} \det(Id_{2E} - S_w(k)) . \quad (33)$$

This function is zero whenever $S_w(k)$ has eigenvalue 1, the prefactor is always nonzero because $S_w(k)$ is unitary. It is inserted to make $\zeta_w(k)$ real on the real axis.

To prove theorem 1.2 one observes first that the function ζ_w can be extended holomorphically in k into a neighbourhood of the real line because the end values $\psi^\pm(L)$ depend holomorphically on k , [PT87]. Moreover, by the Schwarz reflection principle, the function $\zeta_w(k)$ satisfies

$$\zeta_w(\overline{k}) = \overline{\zeta_w(k)}. \quad (34)$$

The spectral density is derived using the Cauchy argument principle. Let $\{k_n^2\}_n$ denote the sequence of positive eigenvalues. In order to expand the spectral density into a sum of periodic orbits, the matrix $S_w(k)$ needs to be subunitary above the real axis. By lemma 2.3 this is only true for k sufficiently large, therefore only eigenvalues larger than some constant K are counted. Negative eigenvalues, ie imaginary values of k are also ignored. Assume K^2 is not an eigenvalue. Let

$$C_{\varepsilon,K} := \{z \in \mathbb{C} \mid -\varepsilon \leq \operatorname{Im}(z) \leq \varepsilon, \operatorname{Re}(z) > K\} \quad (35)$$

and let φ be a test function, then

$$\begin{aligned} \sum_{k_n > K}^\infty \varphi(k_n) &= \frac{1}{2\pi i} \lim_{\varepsilon \rightarrow 0} \int_{\partial C_{\varepsilon,K}} \varphi(k) \frac{\partial}{\partial k} \ln(\zeta_w(k)) dk \\ &= -\frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \operatorname{Im} \int_K^\infty \varphi(k + i\varepsilon) \frac{\partial}{\partial k} \ln(\zeta_w(k + i\varepsilon)) dk \end{aligned} \quad (36)$$

where we used the Schwartz reflection principle. The integral over the interval $(-\varepsilon, \varepsilon)$ vanishes in the limit $\varepsilon \rightarrow 0$ because K^2 is not an eigenvalue.

Plugging in the definition of $\zeta_w(k)$ gives

$$\begin{aligned} \sum_{k_n > K}^\infty \varphi(k_n) &= \frac{1}{2\pi} \operatorname{Im} \int_K^\infty \varphi(k) \frac{\partial}{\partial k} \ln(\det S_w(k)) dk \\ &\quad - \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \operatorname{Im} \int_K^\infty \varphi(k + i\varepsilon) \frac{\partial}{\partial k} \ln \det(I d_{2E} - S_w(k + i\varepsilon)) dk \end{aligned} \quad (37)$$

In the first integral the limit $\varepsilon \rightarrow 0$ commutes with the integral because $S_w(k)$ is unitary and thus the function inside the integral does not have any poles on the real axis.

Let $\Theta_w(k) = \frac{1}{i} \ln \det T(k; w)$, then $\Theta_w(k)$ is real on the real axis because $T(k; w)$ is unitary. Then

$$\frac{\partial}{\partial k} \ln(\det S_w(k)) = i \frac{\partial \Theta_w(k)}{\partial k} \quad (38)$$

because Σ is k -independent.

If K is sufficiently large, by lemma 2.3, the matrix S_w is subunitary above the real axis, so it admits the expansion

$$\ln(\det(I d_{2E} - S_w(k + i\varepsilon))) = - \sum_{n=1}^\infty \frac{1}{n} \operatorname{tr}(S_w^n(k + i\varepsilon)) \quad (39)$$

This gives

$$\begin{aligned} \sum_{k_n > K}^{\infty} \varphi(k_n) &= \frac{1}{2\pi} \int_K^{\infty} \varphi(k) \frac{\partial \Theta_w(k)}{\partial k} dk \\ &\quad + \frac{1}{\pi} \lim_{\varepsilon \rightarrow 0} \operatorname{Im} \int_K^{\infty} \varphi(k + i\varepsilon) \frac{\partial}{\partial k} \sum_{n=1}^{\infty} \frac{1}{n} \operatorname{tr}(S_w^n(k + i\varepsilon)) dk \end{aligned} \quad (40)$$

The $\operatorname{tr}(S_w^n)$ terms can be interpreted as a sum over periodic orbits by using the identity.

$$\sum_{n=1}^{\infty} \frac{\operatorname{tr}(\Sigma T(k; w))^n}{n} = \sum_{n=1}^{\infty} \frac{1}{2n} \operatorname{tr} \begin{pmatrix} 0 & \Sigma \\ T(k; w) & 0 \end{pmatrix}^{2n} \quad (41)$$

Each edge in the original quantum graph is seen as a scatterer with scattering matrix given by the transition matrix $t^{(e)}(k; w_e)$ corresponding to the potential on that edge. Thus the $\operatorname{tr}(S_w(k)^n)$ terms are counting the periodic orbits of the bipartite graph \mathcal{G}^* built from the original graph \mathcal{G} by inserting an extra vertex on each edge. Let PO^* denote the set of periodic orbits of \mathcal{G}^* , $p \in PO^*$. Let n_p be the topological length of the periodic orbit p , that is the number of edges it traverses. Denote by \tilde{p} the primitive periodic orbit that p is a repetition of. Then

$$\operatorname{Im} \frac{\partial}{\partial k} \sum_{n=1}^{\infty} \frac{1}{n} \operatorname{tr}(S_w(k)^n) = \sum_{n=1}^{\infty} \frac{1}{n} \sum_{p \in PO^*, n_p = n} n_{\tilde{p}} \operatorname{Im} \frac{\partial}{\partial k} \prod_{d \in p} \tau_{dd'}(k) \quad (42)$$

Here d' is the bond that follows d in p . The coefficients $\tau_{dd'}(k)$ are of two different types. If the vertex between them is a vertex v of the original graph then $\tau_{dd'}(k) = \sigma_{dd'}^{(v)}$ is the vertex scattering coefficient at that vertex from the Σ matrix, (which is independent of k). If the vertex between them corresponds to one of the edges e of the original graph, then $\tau_{dd'}(k) = t_{dd'}^{(e)}(k)$ from the corresponding edge transition matrix.

The factor $n_{\tilde{p}}$ comes from the fact that each periodic orbit is counted once for each starting vertex.

Theorem 1.2 follows once we identify

$$\mathcal{A}_p(k) = \frac{n_{\tilde{p}}}{n_p} \operatorname{Im} \frac{\partial}{\partial k} \prod_{d \in p} \tau_{dd'}(k) \quad (43)$$

The trace formula can also be written in distribution form

$$\sum_{k_n > K}^{\infty} \delta_{k_n}(k) = \frac{1}{2\pi} \frac{\partial \Theta_w(k)}{\partial k} + \frac{1}{\pi} \sum_{p \in PO^*} \mathcal{A}_p(k) \quad (44)$$

4. Example – edges dressed with δ -potentials

To illustrate the formal results, we discuss here a graph dressed with δ -potential on the edges. The solutions ψ^{\pm} are explicit so one can write down an explicit trace formula. This example shows clearly how an edge with a potential acts as a scatterer. Note that a δ -potential can also be modelled by introducing a vertex with suitable boundary conditions, there is an exact trace formula for these cases, see [KS99b] or [BE09]. The results here recover the ones in these two papers.

First consider a single edge parametrized as $[0, L]$, look at

$$-\psi''(x) + D\delta_{x_0}(x)\psi(x) = k^2\psi(x) \quad (45)$$

This implies that ψ' has a jump discontinuity at x_0 namely

$$\lim_{\varepsilon \rightarrow 0}(\psi'(x_0 + \varepsilon) - \psi'(x_0 - \varepsilon)) = D\psi(x_0) \quad (46)$$

Here D is some real parameter that measures the magnitude and $x_0 \in [0, L]$ is the location of the δ -potential.

Assume for now that k is real, so only positive eigenvalues are considered. The two individual solutions are then of the form

$$\begin{aligned} \psi^+(x) &= \begin{cases} e^{-ikx} & x < x_0 \\ \frac{D}{2ik}e^{-2ikx_0}e^{ikx} + (1 - \frac{D}{2ik})e^{-ikx} & x > x_0 \end{cases} \\ \psi^-(x) &= \begin{cases} e^{ikx} & x < x_0 \\ (1 + \frac{D}{2ik})e^{ikx} - \frac{D}{2ik}e^{2ikx_0}e^{-ikx} & x > x_0 \end{cases} \end{aligned} \quad (47)$$

where the coefficients in the linear combination were computed from the continuity of the solutions and the jump in their derivatives.

The Wronskian is then $W(\psi^+, \psi^-) = 2ik$ on the entire edge. In terms of the edge \hat{d} with reverse orientation the δ -potential is situated at $L - x_0$, so the transition matrix is

$$t(k, D\delta_{x_0}) = \frac{1}{(1 - \frac{D}{2ik})e^{-ikL}} \begin{pmatrix} 1 & \frac{D}{2ik}e^{-2ikx_0}e^{ikL} \\ \frac{D}{2ik}e^{2ikx_0}e^{-ikL} & 1 \end{pmatrix} \quad (48)$$

with eigenvalues

$$\mu_1(k) = e^{ikL} \quad \mu_2(k) = \frac{2ik + D}{2ik - D}e^{ikL} \quad (49)$$

Lemma 4.1.

If the δ -potential is positive, $D \geq 0$, the matrix $t(k + i\varepsilon; D\delta_{x_0})$ is subunitary for all real k . If $D < 0$ it is only subunitary for sufficiently large values of k , namely for

$$k^2 > -\frac{D}{L} - \frac{D^2}{4} \quad (50)$$

Proof. Let $\varepsilon > 0$ then

$$\mu_1(k + i\varepsilon) = e^{ikL}e^{-\varepsilon L} \quad (51)$$

so

$$|\mu_1(k + i\varepsilon)| < |\mu_1(k)| = 1 \quad (52)$$

For the second eigenvalue

$$\mu_2(k + i\varepsilon) = \frac{2ik - 2\varepsilon + D}{2ik - 2\varepsilon - D}e^{ikL}e^{-\varepsilon L} \quad (53)$$

thus

$$\frac{d}{d\varepsilon} |\mu_2(k + i\varepsilon)|^2 \Big|_{\varepsilon=0} = -\frac{8D}{D^2 + 4k^2} - 2L \quad (54)$$

which means

$$|\mu_2(k + i\varepsilon)| < 1 \quad \Leftrightarrow \quad L > \frac{-D}{(D/2)^2 + k^2} \quad (55)$$

This is trivially satisfied if $D \geq 0$ but not true in general if $D < 0$. \square

Remark 4.2.

The matrix $t(k; D\delta_{x_0})$ is only subunitary above the real axis for large enough values of k . This is the same situation as in lemma 2.3 for potentials in $L^2([0, L])$.

The trace formula contains terms of the form $\frac{\partial}{\partial k} \ln \det t(k; D\delta_{x_0})$ which can be explicitly computed using

$$\mu_1(k) = e^{ikL} \quad \mu_2(k) = \frac{2ik + D}{2ik - D} e^{ikL} = e^{-2i \arctan(\frac{D}{2k}) + ikL} \quad (56)$$

so that

$$\frac{1}{i} \frac{\partial}{\partial k} \ln \det t(\delta; k) = 2L + \frac{2D}{4k^2 + D^2} \quad (57)$$

Corollary 4.3.

The trace formula with a δ -potential of strength D_e on each edge reads

$$\sum_{k_n > K}^{\infty} \delta_{k_n}(k) = \frac{\mathcal{L}}{\pi} + \frac{1}{\pi} \sum_{e=1}^E \frac{D_e}{4k^2 + D_e^2} + \frac{1}{\pi} \sum_{p \in PO^*} \mathcal{A}_p(k) \quad (58)$$

with coefficients

$$\mathcal{A}_p(k) = \frac{n_{\tilde{p}}}{n_p} \operatorname{Im} \frac{\partial}{\partial k} \prod_{d \in p} \tau_{dd'}(k) \quad (59)$$

and the $\tau_{dd'}(k)$ from the matrix $\Sigma T(k; D\delta_{x_0})$ with $t^{(e)}(k; D_e\delta_{x_0})$ computed above in equation 48. Here K has to be chosen so that the inequality in lemma 4.1 is satisfied on all edges.

5. The high-energy limit

Consider the high-energy limit, that is, assume that k is real and $k^2 \gg \|w\|_{L^\infty(G)}$. The exact solutions will be approximated by the WKB-method. This requires some estimates on the WKB approximation so the main steps in its derivation will be recalled. The goal is to find an approximate solution to

$$-\psi''(x) + w(x)\psi(x) = k^2\psi(x) \quad (60)$$

for large values of k . Set

$$p(x) := \sqrt{k^2 - w(x)} \quad s(x) := \int_0^x p(x') dx' \quad (61)$$

and then use the substitution

$$\psi(x) =: p^{-1/2}(x)\eta(s(x)) \quad (62)$$

This is well defined as $p(x) > 0$ by the assumptions. The equation then transforms to

$$\frac{\partial^2}{\partial s^2}\eta(s) + \eta(s) = - \left(\frac{1}{4}w''(x(s))p^{-4}(x(s)) + \frac{5}{16}w'(x(s))^2p^{-6}(x(s)) \right) \eta(s) \quad (63)$$

Let $\chi(x) := \frac{1}{4}w''(x)p^{-4}(x) + \frac{5}{16}w'(x)^2p^{-6}(x)$ to simplify notation. Equation (63) is solved iteratively by a power series $\eta(s) := \sum_{j=0} \eta_j(s)$. The two initial solutions are $\eta_0(s) := e^{\pm is}$ and the general term is the solution of

$$\frac{\partial^2}{\partial s^2}\eta_j(s) + \eta_j(s) = -\chi(x(s))\eta_{j-1}(s) \quad (64)$$

This is a second order linear differential equation which can be solved explicitly through variation of constants.

$$\eta_j(s) = -e^{is} \int_0^s e^{-2is'} \int_0^{s'} e^{is''} \chi(x(s'')) \eta_{j-1}(s'') ds'' ds' \quad (65)$$

This process converges if χ is sufficiently small, which is satisfied for k sufficiently large. The WKB-approximation is simply η_0 , written in the x variable this yields the familiar

$$\psi_{WKB}^{\pm}(x) := \sqrt{\frac{p(0)}{p(x)}} e^{\mp i \int_0^x p(x') dx'} \quad (66)$$

where the constant $\sqrt{p(0)}$ term was inserted for normalization.

Lemma 5.1.

On each edge the WKB-solutions differ from the exact solutions by an error term that decays like k^{-2} for k sufficiently large.

$$\begin{aligned} |\psi^{\pm}(x) - \psi_{WKB}^{\pm}(x)| &< \frac{C}{k^2} \\ |(\psi^{\pm})'(x) - (\psi_{WKB}^{\pm})'(x)| &< \frac{C}{k} \end{aligned} \quad (67)$$

with C independent of k and $x \in [0, L]$.

Proof. For k large, $p(x) \sim k$ so $s(x) \sim k$ and $\chi(x) \sim k^{-4}$. The iteration then gives $\eta_j(x) \sim k^{-2j}$ and $(\eta_j)'(x) \sim k^{-2j+1}$ so the results follow from

$$\psi^{\pm}(x) - \psi_{WKB}^{\pm}(x) = \sum_{j=1} \eta_j(x) \quad (68)$$

□

On top of approximating the exact solution by the WKB-solution, the derivatives of the WKB-solution will be approximated as follows.

$$(\psi_{WKB}^{\pm})'(x) = \mp ik \psi_{WKB}^{\pm}(x) + O(k^{-1}) \quad (69)$$

Thus

$$\psi_{WKB}^{\pm}(0) = 1 \quad (\psi_{WKB}^{\pm})'(0) = \mp ik + O(k^{-1}) \quad (70)$$

Both layers of approximation have an error term that is two orders smaller than the main term.

The transition matrix for the WKB-approximation can now be computed explicitly.

$$\begin{aligned} & t(k; w) \\ &= t^{WKB}(k; w) + O(k^{-2}) \\ &= \begin{pmatrix} (\psi_{WKB}^+(L))^{-1} & 0 \\ 0 & (\psi_{WKB}^-(L))^{-1} \end{pmatrix} + O(k^{-2}) \\ &= \begin{pmatrix} e^{i \int_0^L p(x) dx} & 0 \\ 0 & e^{i \int_0^L p(x) dx} \end{pmatrix} + O(k^{-2}) \end{aligned} \quad (71)$$

This information will now be used to study the behaviour of the trace formula in the high energy limit. Notice that the function s defined in (61), now seen as a function of k , corresponds to the classical action along an edge of the graph:

$$s_d(k) = s_{\hat{d}}(k) := \int_0^{L_d} \sqrt{k^2 - w_d(x)} dx \quad (72)$$

Recall that $\Theta_w(k) = \frac{1}{i} \ln \det T(k; w)$, which can be approximated to $O(k^{-2})$ by

$$\Theta_w(k) = \Theta_w^{WKB}(k) + O(k^{-2}) = \sum_{d \in \mathcal{D}} s_d(k) + O(k^{-2}) \quad (73)$$

Note that the trace formula as stated in equation (13) contains the derivative of the $\Theta_w(k)$, which in the WKB approximation reads

$$\frac{\partial}{\partial k} \Theta_w^{WKB}(k) = \sum_{d \in \mathcal{D}} \int_0^{L_d} \frac{k dx}{\sqrt{k^2 - w_d(x)}} + \frac{\partial}{\partial k} O(k^{-2}). \quad (74)$$

Each of the integrals above can be identified as the time it takes a particle to traverse the edge (in the system of units used here, “time” is expressed in units of length). In the physics literature, the derivative of Θ_w is known as the Wigner delay time which will be denoted here by $\mathcal{T}(k)$. The result above can be interpreted as the Wigner delay time for a graph. In the high energy limit, it approaches the total length of the graph.

An important consequence of the WKB approximation to the edge transition matrix (71) is that reflections by the edge potential can be neglected to order $\frac{1}{k^2}$. This fact allows us to neglect the contribution to the trace formula from all the periodic orbits in the graph that involve a reflection on an edge. In other words, only the periodic orbits from the original graph \mathcal{G} survive. Their weights $\mathcal{A}_p(k)$ split into a vertex scattering part and the contribution from the edges.

$$\mathcal{A}_p(k) = \mathcal{A}_p^{WKB}(k) + \frac{\partial}{\partial k} O(k^{-2}). \quad (75)$$

and

$$\mathcal{A}_p^{WKB}(k) = \frac{\partial}{\partial k} \left(\frac{n_{\bar{p}}}{n_p} \text{Im} \prod_{v \in p} \sigma_{dd'}^v \prod_{d \in p} e^{i \int_0^{L_d} \sqrt{k^2 - w_d(x)} dx} \right) \quad (76)$$

Here the $\sigma_{dd'}^v = -\delta_{bb'} + \frac{2}{\deg(v)}$ are from the Kirchhoff-Neumann boundary conditions as before. To cast the trace formula in a form similar to the semi-classical trace formula [Gut90], it is convenient to define the following quantities for each periodic orbit of topological length n_p which consists of r_p repetitions of a primitive periodic orbit of length $n_{\bar{p}}$:

Let $A_{\bar{p}} = |\prod_{v \in \bar{p}} \sigma_{dd'}^v|$ and let $\nu_{\bar{p}}$ be the number of back scatters (where $\sigma_{dd'}^v < 0$). Let $S_{\bar{p}}(k) = \sum_{d \in \bar{p}} s_d(k)$ which is the classical action along the periodic orbit, and let $T_{\bar{p}}(k) = \frac{\partial}{\partial k} S_{\bar{p}}(k)$ denote the classical period. Then,

$$\mathcal{A}_p^{WKB}(k) = T_{\bar{p}}(k) A_{\bar{p}}^{r_p} \cos((S_{\bar{p}}(k) + \pi \nu_{\bar{p}}) r_p) . \quad (77)$$

The analogy with the Gutzwiller trace formula is completed when $A_{\bar{p}}^2$ is identified as the classical probability to survive along the period orbit, and $\nu_{\bar{p}}$ the index replacing the Maslov index. Again to zeroth order this simplifies to the no potential situation.

Finally,

$$\begin{aligned} \sum_{k_n > K}^{\infty} \varphi(k_n) &= \frac{1}{2\pi} \int_K^{\infty} \varphi(k) \mathcal{T}(k) dk \\ &+ \frac{1}{\pi} \int_K^{\infty} \varphi(k) \sum_{p \in PO} T_{\bar{p}}(k) A_{\bar{p}}^{r_p} \cos((S_{\bar{p}}(k) + \pi \nu_{\bar{p}}) r_p) dk \\ &+ \int_K^{\infty} \varphi(k) \frac{\partial}{\partial k} E(k) dk \end{aligned} \quad (78)$$

where $E(k)$ is the error term, it decays as $E(k) = O(k^{-2})$.

Remark 5.2.

Note that the term involving the Euler characteristic from the classic trace formula is not visible because the formula here is only valid for large values of k and this term would appear as a δ distribution located at $k = 0$.

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References

- [BE08] Jens Bolte and Sebastian Endres, *Trace formulae for quantum graphs*, Analysis on graphs and its applications, Proc. Sympos. Pure Math., vol. 77, Amer. Math. Soc., Providence, RI, 2008, pp. 247–259.
- [BE09] ———, *The trace formula for quantum graphs with general self adjoint boundary conditions*, Ann. Henri Poincaré **10** (2009), no. 1, 189–223.
- [CS07] V. L. Chernyshev and A. I. Shafarevich, *The semiclassical spectrum of the Schrödinger operator on a geometric graph*, Math. Notes **82** (2007), no. 3-4, 542–554.

- [GS06] Sven Gnutzmann and Uzy Smilansky, *Quantum graphs: Applications to quantum chaos and universal spectral statistics*, *Advances in Physics* **55** (2006), 527–625.
- [Gut90] Martin C. Gutzwiller, *Chaos in classical and quantum mechanics*, Interdisciplinary Applied Mathematics, vol. 1, Springer-Verlag, New York, 1990.
- [HKT12] J M Harrison, K Kirsten, and C Texier, *Spectral determinants and zeta functions of Schrödinger operators on metric graphs*, *J. Phys. A* **45** (2012), no. 12, 125206.
- [KPS07] Vadim Kostrykin, Jürgen Potthoff, and Robert Schrader, *Heat kernels on metric graphs and a trace formula*, *Adventures in mathematical physics*, *Contemp. Math.*, vol. 447, Amer. Math. Soc., Providence, RI, 2007, pp. 175–198.
- [KS97] Tsampikos Kottos and Uzy Smilansky, *Quantum chaos on graphs*, *Physical Review Letters* **79** (1997), 4794–4797.
- [KS99a] V. Kostrykin and R. Schrader, *Kirchhoff’s rule for quantum wires*, *J. Phys. A* **32** (1999), no. 4, 595–630.
- [KS99b] Tsampikos Kottos and Uzy Smilansky, *Periodic orbit theory and spectral statistics for quantum graphs*, *Ann. Physics* **274** (1999), no. 1, 76–124.
- [Kuc08] Peter Kuchment, *Quantum graphs: an introduction and a brief survey*, *Analysis on graphs and its applications*, *Proc. Sympos. Pure Math.*, vol. 77, Amer. Math. Soc., Providence, RI, 2008, pp. 291–312.
- [Pos09] Olaf Post, *First order approach and index theorems for discrete and metric graphs*, *Ann. Henri Poincaré* **10** (2009), no. 5, 823–866.
- [PT87] Jürgen Pöschel and Eugene Trubowitz, *Inverse spectral theory*, *Pure and Applied Mathematics*, vol. 130, Academic Press Inc., Boston, MA, 1987.
- [Rot84] Jean-Pierre Roth, *Le spectre du laplacien sur un graphe*, *Théorie du potentiel* (Orsay, 1983), *Lecture Notes in Math.*, vol. 1096, Springer, Berlin, 1984, pp. 521–539.